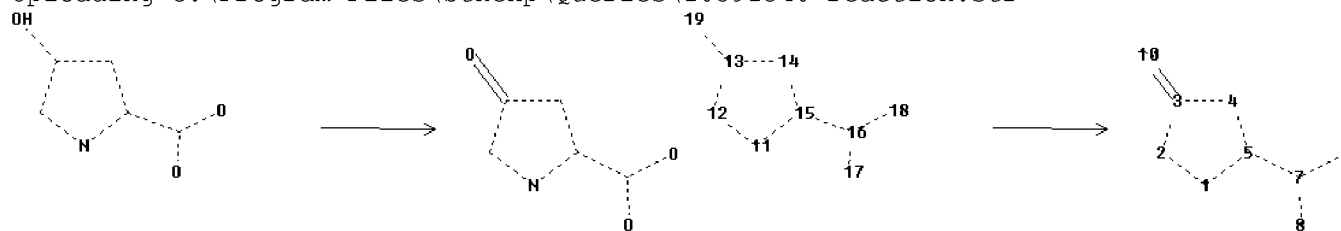


=>

Uploading C:\Program Files\Stnexp\Queries\10591340-reaction.str



chain nodes :

7 8 9 10 16 17 18 19

ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

3-10 5-7 7-8 7-9 13-19 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 2-3 3-4 3-10 4-5 5-7 7-8 7-9 11-12 11-15 12-13 13-14 13-19

14-15 15-16 16-17 16-18

isolated ring systems :

containing 1 : 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 11

node mappings:

7:16 5:15 4:14 3:13 2:12 1:11 8:17 9:18

L1 STRUCTURE UPLOADED

=> s l1 sss full

FULL SEARCH INITIATED 16:25:59 FILE 'CASREACT'

SCREENING COMPLETE - 26248 REACTIONS TO VERIFY FROM 1329 DOCUMENTS

100.0% DONE 26248 VERIFIED 150 HIT RXNS (4 INCOMP) 60 DOCS

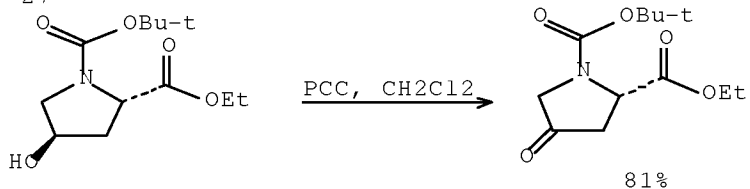
SEARCH TIME: 00.00.02

L3 60 SEA SSS FUL L1 (150 REACTIONS)

=> d tot

L3 ANSWER 1 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

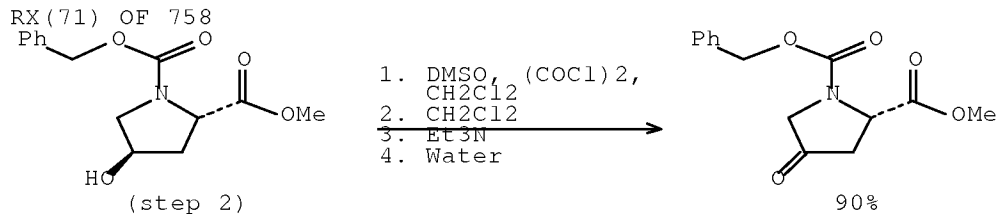
RX(3) OF 27



REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 101092383, 26 Dec 2007
CON: 12 hours, reflux

L3 ANSWER 2 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

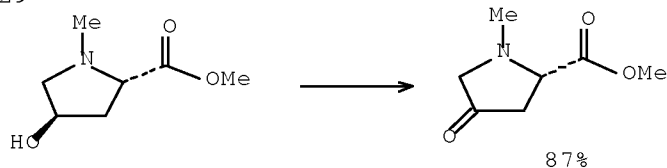
RX(71) OF 758



(step 2)
REF: Journal of Medicinal Chemistry, 50(20), 4953-4975; 2007
CON: STAGE(1) 15 minutes, -78 deg C
STAGE(2) 30 minutes, -78 deg C
STAGE(3) -78 deg C -> room temperature
STAGE(4) room temperature

L3 ANSWER 3 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

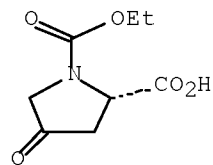
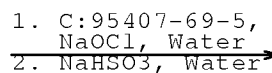
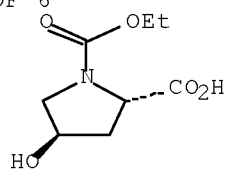
RX(3) OF 129



REF: Tetrahedron Letters, 48(27), 4691-4694; 2007
NOTE: no experimental detail, Swern oxidation

L3 ANSWER 4 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 6



(step 1)

90%

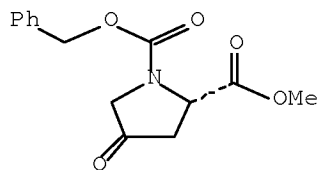
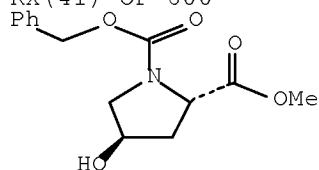
REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1939904, 04 Apr 2007

NOTE: solvent not specified, green chem.-catalyst

CON: 5 - 300 minutes, -25 - 100 deg C

L3 ANSWER 5 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(41) OF 600



(step 1)

58%

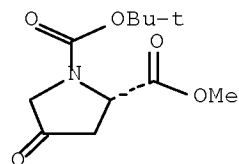
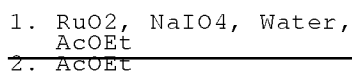
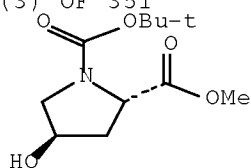
REF: Bioorganic & Medicinal Chemistry, 15(7), 2631-2650; 2007

CON: STAGE(1) 0 deg C; 88 hours, room temperature

STAGE(2) room temperature

L3 ANSWER 6 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 351

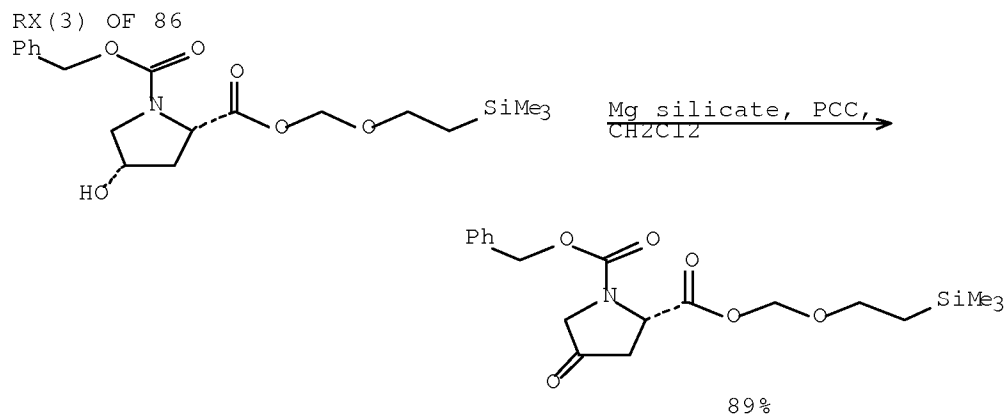


(step 2)

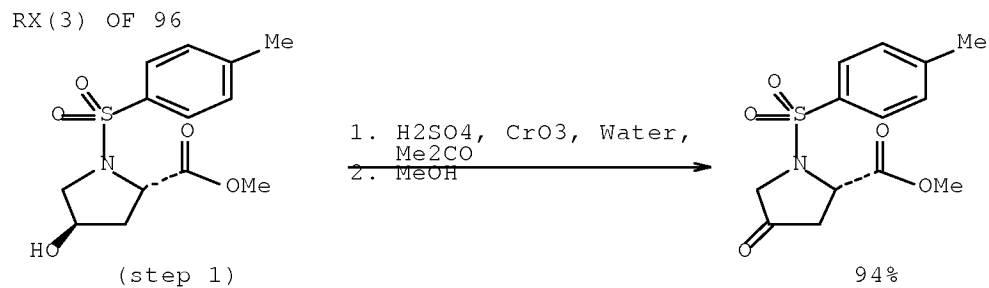
94%

REF: Journal of Combinatorial Chemistry, 9(1), 143-157; 2007

CON: STAGE(2) 0 deg C; 15 hours, 0 deg C -> room temperature

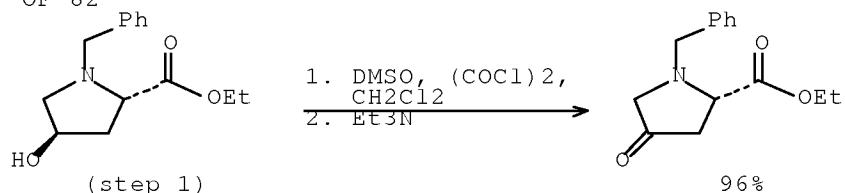


REF: Tetrahedron: Asymmetry, 17(17), 2479-2486; 2006
 NOTE: optimized on oxidation conditions, optimization study
 CON: 16 hours, room temperature



REF: Zhongguo Yiyao Gongye Zazhi, 36(3), 129-132; 2005
 CON: STAGE(1) cooled; 2 hours
 STAGE(2) 15 minutes

RX(5) OF 82



REF: Bioorganic & Medicinal Chemistry Letters, 16(18), 4856-4860; 2006

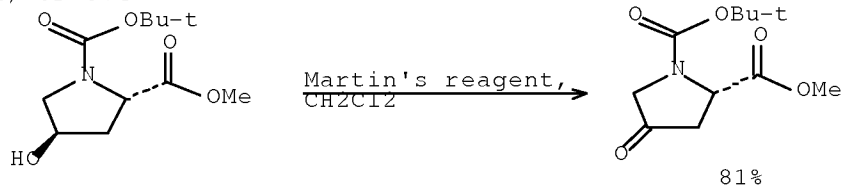
NOTE: Swern oxidation

CON: STAGE(1) -78 deg C

STAGE(2) -78 deg C -> room temperature

L3 ANSWER 10 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(24) OF 574

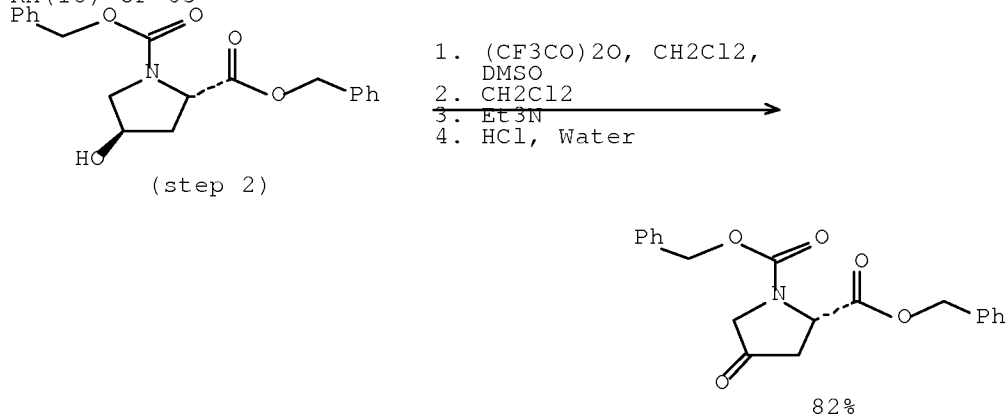


REF: Chemistry--A European Journal, 12(15), 4121-4143; 2006

CON: 1 hour, room temperature

L3 ANSWER 11 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(18) OF 63



REF: Journal of Organic Chemistry, 71(13), 5004-5007; 2006

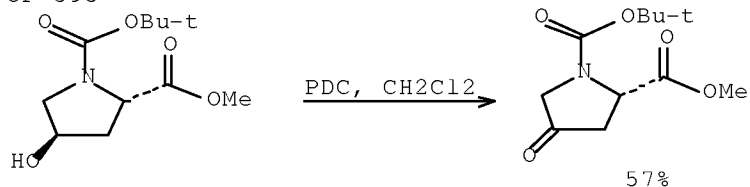
CON: STAGE(1) room temperature -> -78 deg C; 1 hour, -78 deg C

STAGE(2) 2 hours, -78 deg C

STAGE(3) -78 deg C; -78 deg C -> room temperature

L3 ANSWER 12 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

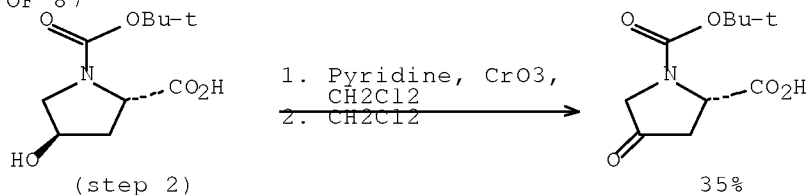
RX(101) OF 395



REF: Bioorganic & Medicinal Chemistry, 14(8), 2725-2746; 2006
CON: 3 days, room temperature

L3 ANSWER 13 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

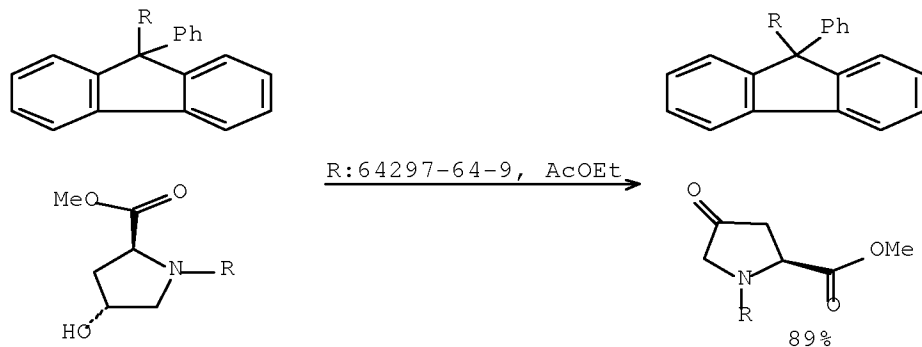
RX(9) OF 87



REF: Bioorganic & Medicinal Chemistry, 14(7), 2253-2265; 2006
CON: STAGE(1) 30 minutes, 0 deg C; 30 minutes, 0 deg C -> room temperature

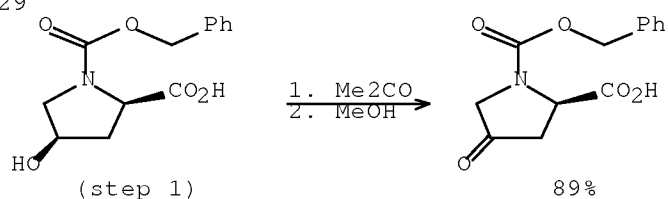
L3 ANSWER 14 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 78



REF: Journal of Organic Chemistry, 70(26), 10860-10863; 2005
CON: reflux

RX(3) OF 129



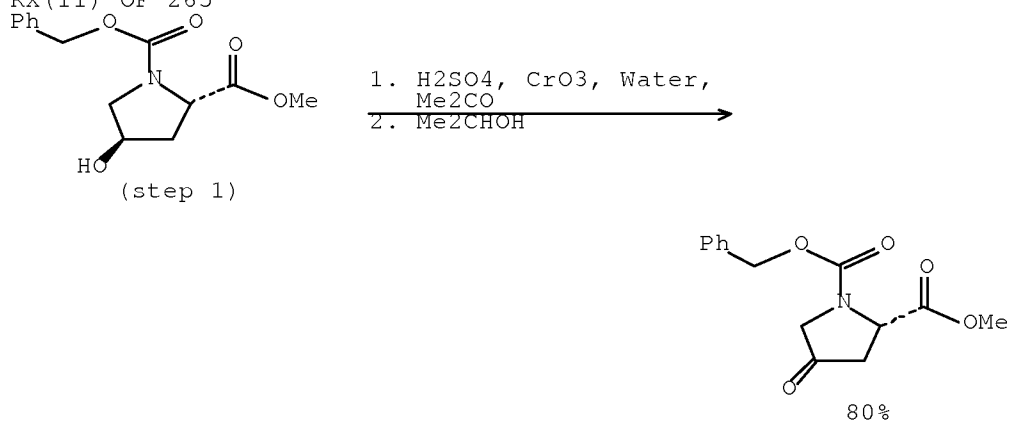
REF: Journal of Organic Chemistry, 70(22), 9002-9008; 2005

NOTE: Jones reagent used in stage 1

CON: STAGE(1) 10 minutes, room temperature; 3 hours, room temperature

STAGE(2) room temperature

RX(11) OF 265

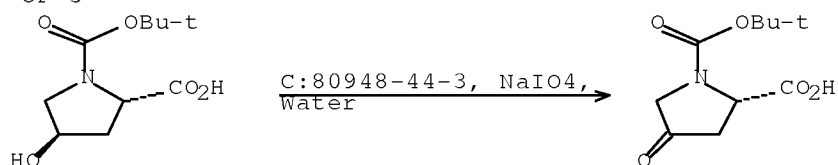


REF: Journal of Medicinal Chemistry, 48(23), 7333-7342; 2005

CON: STAGE(1) 3 minutes, room temperature; 1 hour, room temperature

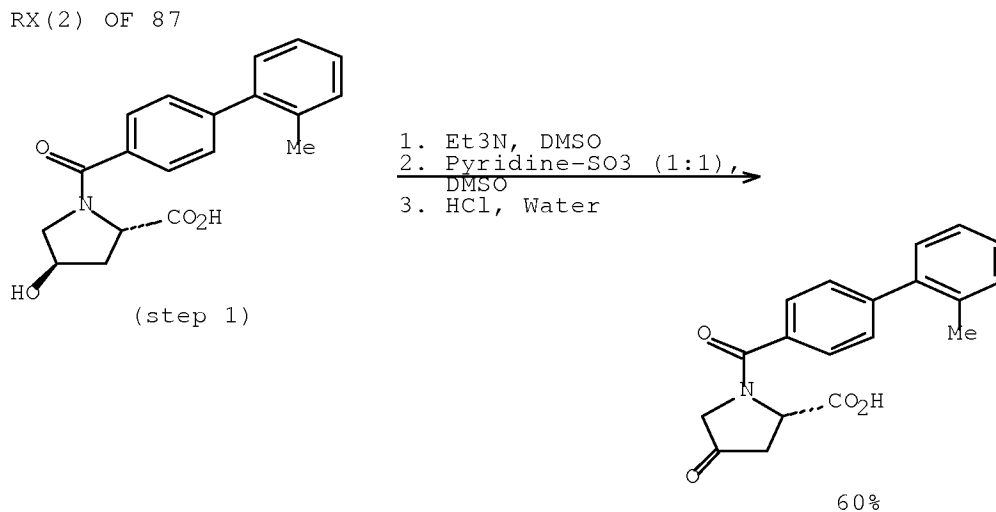
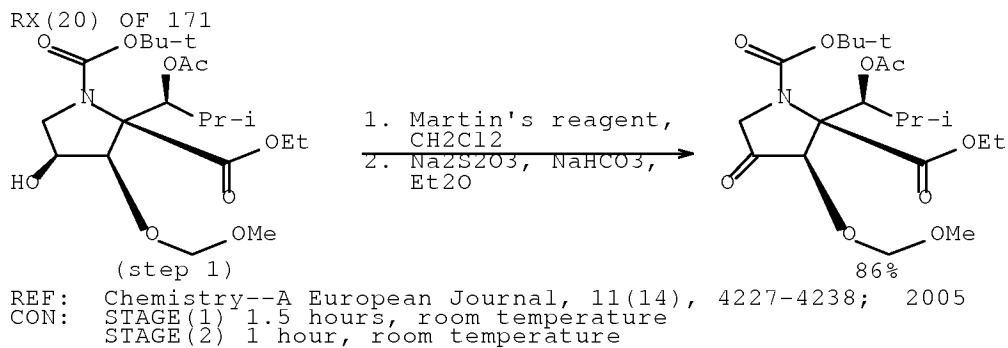
STAGE(2) 20 minutes, room temperature

RX(2) OF 3



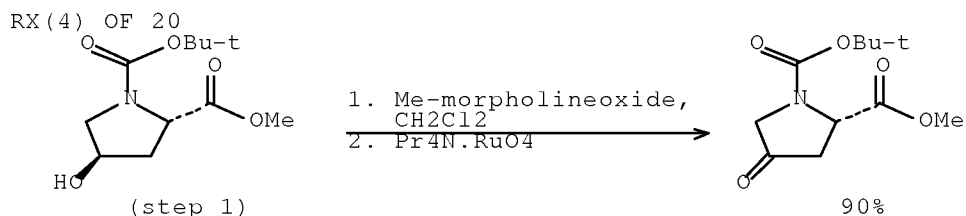
REF: Ger. Offen., 102004010943, 29 Sep 2005

CON: STAGE(1) cooled; 1 - 1.5 hour

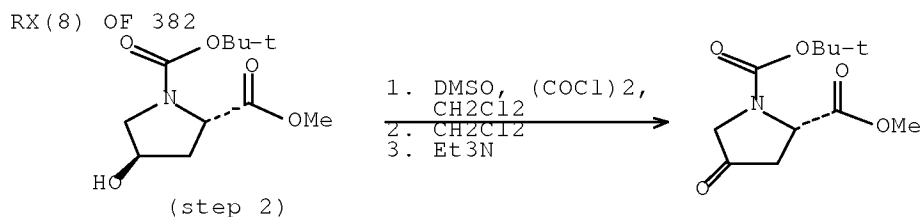


REF: PCT Int. Appl., 2005082848, 09 Sep 2005

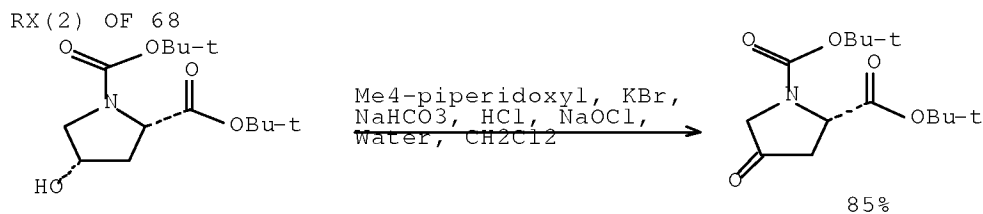
NOTE: workup
CON: STAGE(1) room temperature -> 40 deg C; 40 deg C -> 10 deg C;
5 - 20 deg C
STAGE(2) 5 - 10 minutes; 1 - 3 hour, 15 - 25 deg C;
25 deg C -> 10 deg C
STAGE(3) <30 deg C



REF: Tetrahedron Letters, 46(30), 4985-4987; 2005
 NOTE: green chem.-process simplification, mol. sieves used, other reagent gave somewhat higher yield but less safe reaction
 CON: STAGE(1) 15 minutes, room temperature
 STAGE(2) 5 minutes, room temperature; 210 minutes

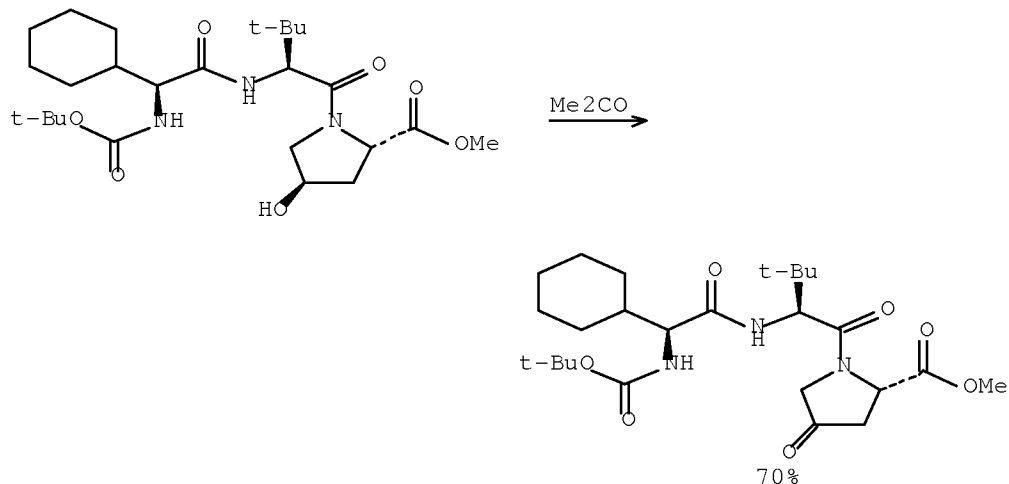


REF: U.S. Pat. Appl. Publ., 20050131019, 16 Jun 2005
 CON: STAGE(1) 5 minutes, room temperature -> -78 deg C
 STAGE(2) 30 minutes, -78 deg C
 STAGE(3) 40 minutes, -78 deg C; 30 minutes, 0 deg C



REF: Tetrahedron, 61(15), 3725-3731; 2005
 NOTE: NaOCl in buffered solution, Aliquat 336 added
 CON: STAGE(1) room temperature -> 0 deg C; 0 deg C

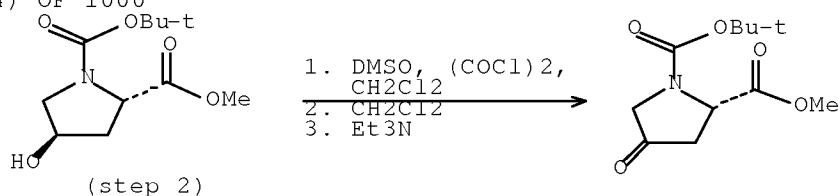
RX(5) OF 51



REF: PCT Int. Appl., 2005037860, 28 Apr 2005
NOTE: Jones reagent used

L3 ANSWER 24 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

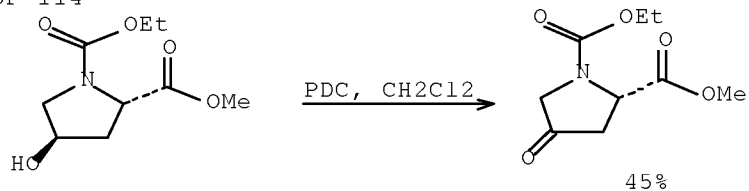
RX(94) OF 1000



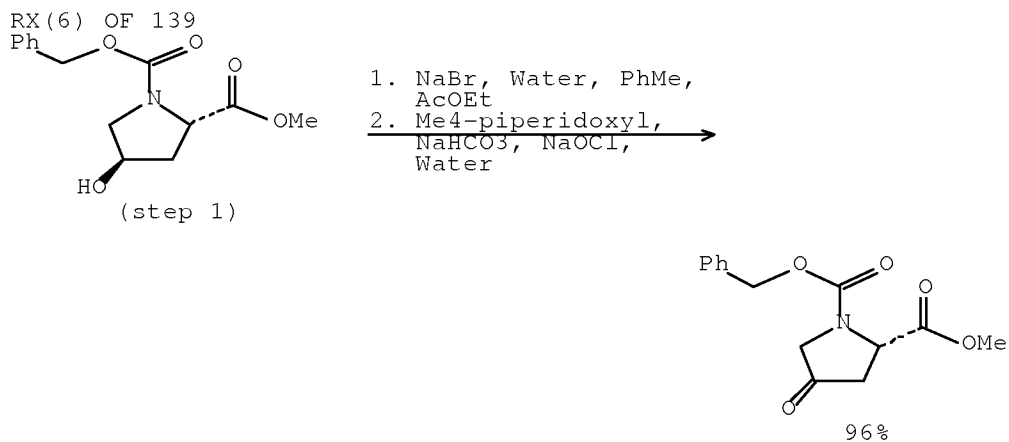
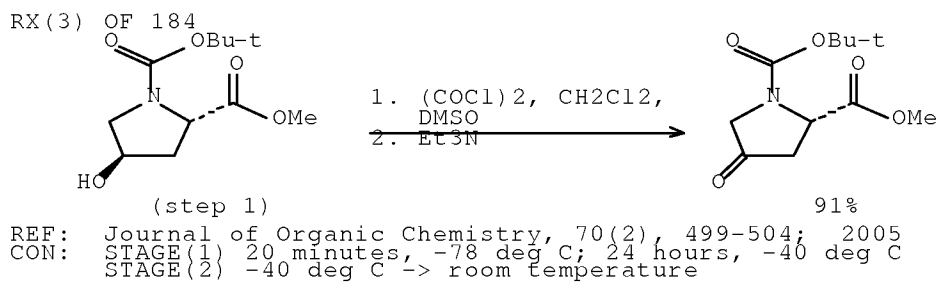
REF: PCT Int. Appl., 2005023762, 17 Mar 2005
CON: STAGE(1) 5 minutes, -78 deg C
STAGE(2) 30 minutes, -78 deg C
STAGE(3) 40 minutes, -78 deg C; 30 minutes, 0 deg C

L3 ANSWER 25 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

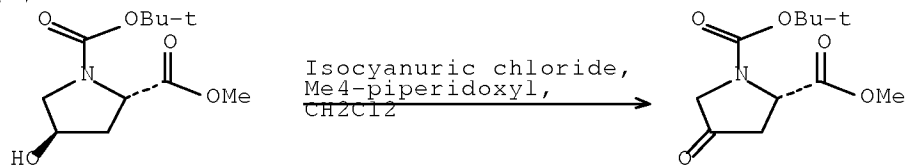
RX(55) OF 114



REF: Journal of Organic Chemistry, 70(3), 898-906; 2005
NOTE: celite used
CON: STAGE(1) 0 deg C; overnight, room temperature



RX(2) OF 145

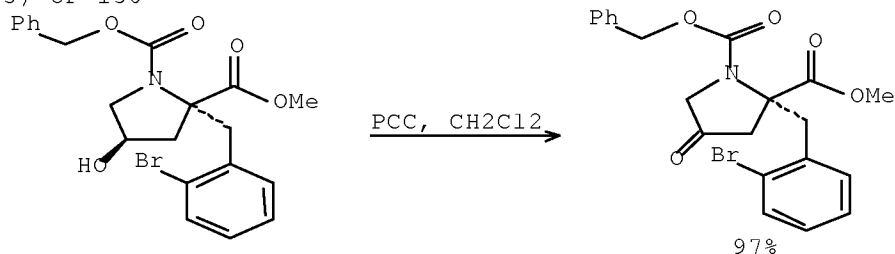


REF: Bioorganic & Medicinal Chemistry Letters, 14(22), 5699-5702;
2004

NOTE: key intermediate

L3 ANSWER 29 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 136



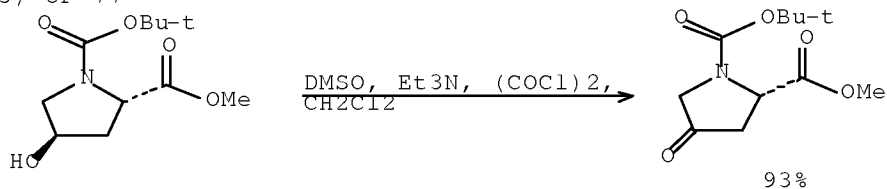
REF: Tetrahedron: Asymmetry, 14(19), 3033-3041; 2003

NOTE: Florisil used

CON: 10 hours, room temperature

L3 ANSWER 30 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 77

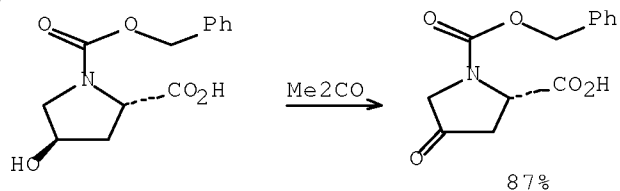


REF: Tetrahedron Letters, 44(42), 7809-7812; 2003

CON: -78 deg C

L3 ANSWER 31 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 120



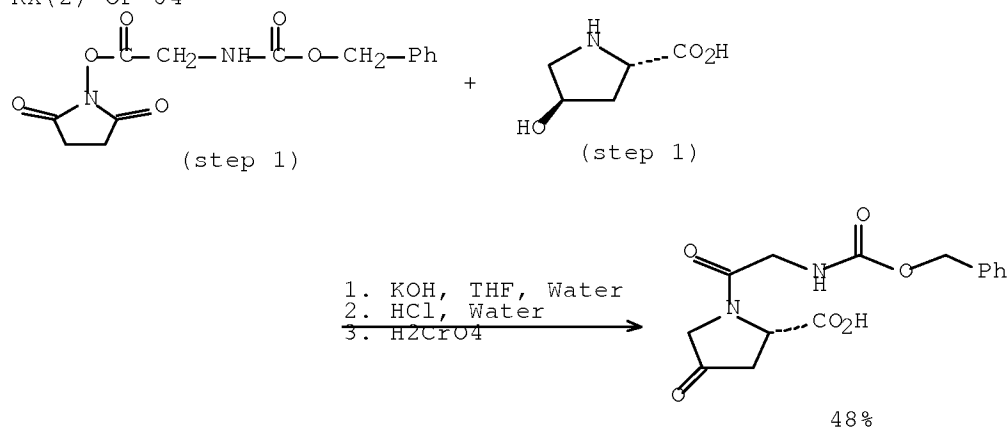
REF: Journal of the American Chemical Society, 125(16), 4702-4703; 2003

NOTE: Jones' reagent used

CON: STAGE(1) 5 minutes, 20 deg C; 30 minutes, 20 deg C

L3 ANSWER 32 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 64



REF: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 28(6), 444-449; 2002

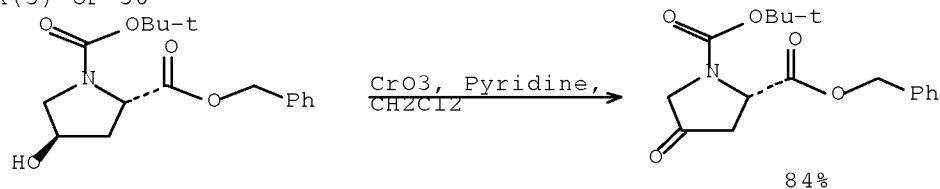
NOTE: literature prepn. stage 3

CON: STAGE(1) 2.5 hours, 20 deg C

STAGE(2) 0 deg C, pH 2 - 3

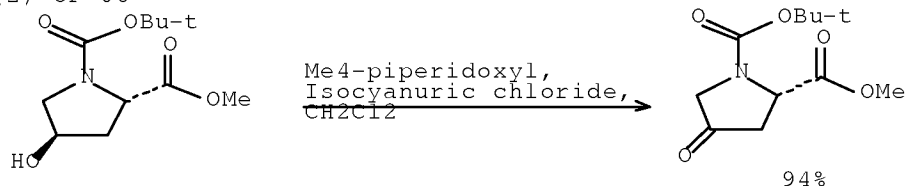
L3 ANSWER 33 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 30



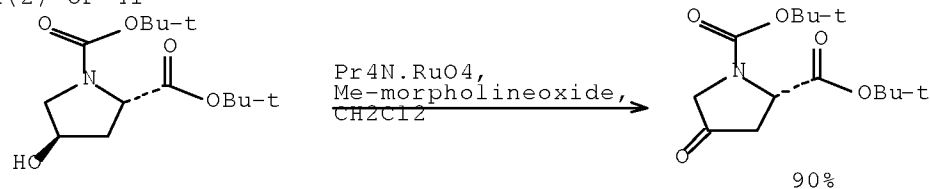
REF: Journal of Organic Chemistry, 67(20), 7162-7164; 2002

RX(2) OF 60



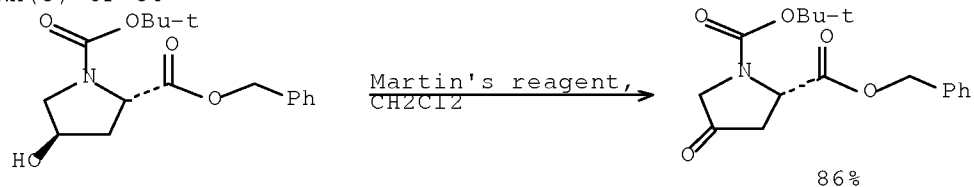
REF: Angewandte Chemie, International Edition, 41(9), 1600-1602;
2002

RX(2) OF 41



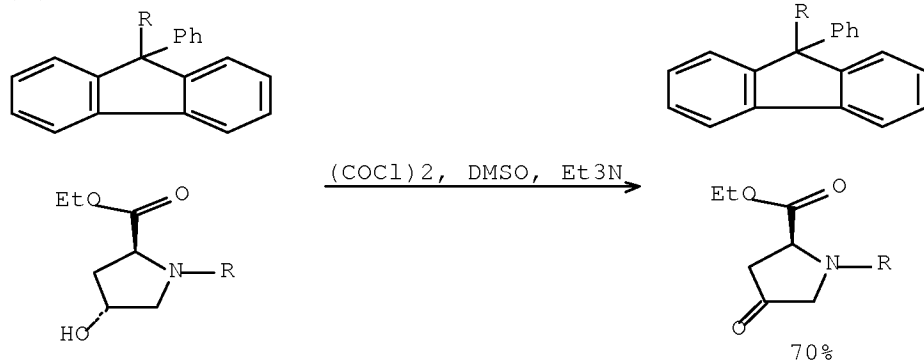
REF: Journal of Organic Chemistry, 66(10), 3593-3596; 2001
NOTE: mol. sieves used

RX(5) OF 36



REF: Synlett, (9), 1465-1467; 1999
NOTE: STEREOSÉLECTIVE

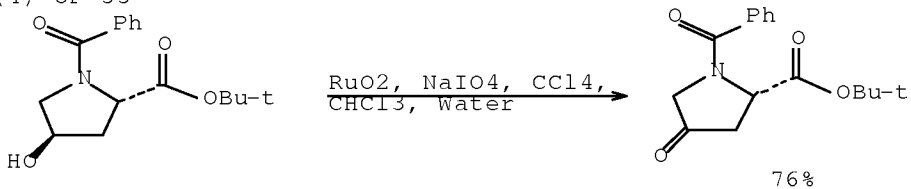
RX(2) OF 14



REF: Tetrahedron Letters, 38(30), 5399-5402; 1997
NOTE: literature ref.

L3 ANSWER 38 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

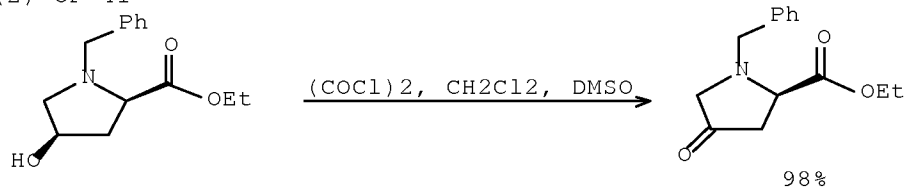
RX(4) OF 55



REF: Tetrahedron, 53(14), 5233-5254; 1997

L3 ANSWER 39 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

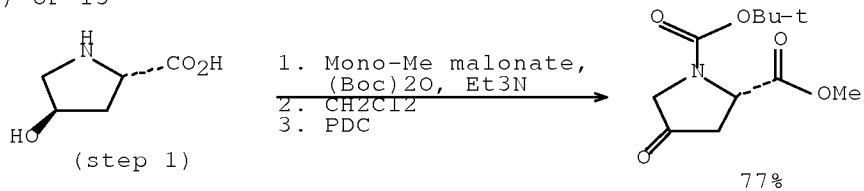
RX(2) OF 41



REF: Journal of Medicinal Chemistry, 39(15), 2990-3000; 1996

L3 ANSWER 40 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

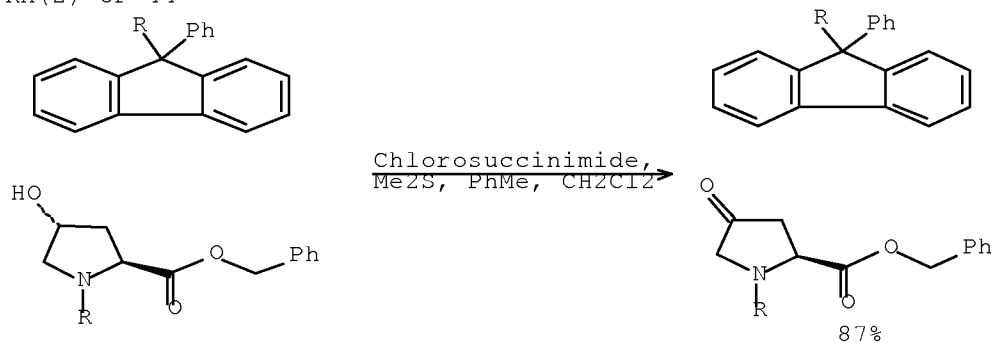
RX(1) OF 15



REF: Synlett, (1), 95-6; 1996

L3 ANSWER 41 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

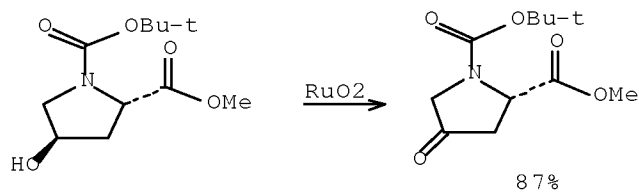
RX(2) OF 44



REF: Journal of Organic Chemistry, 61(1), 202-9; 1996

L3 ANSWER 42 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

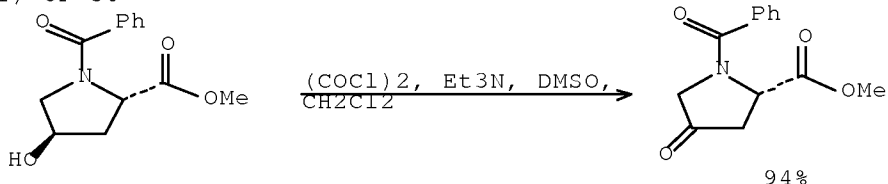
RX(3) OF 26



REF: Chemical & Pharmaceutical Bulletin, 43(10), 1617-20; 1995

L3 ANSWER 43 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

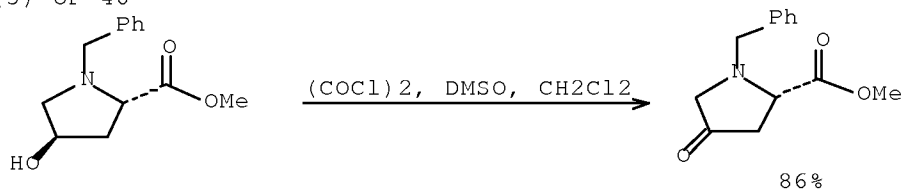
RX(1) OF 56



REF: Chemical & Pharmaceutical Bulletin, 43(8), 1302-6; 1995

L3 ANSWER 44 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

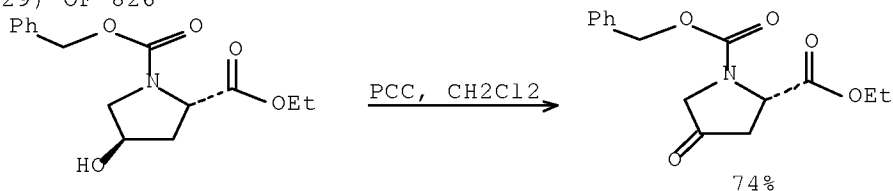
RX(5) OF 46



REF: Tetrahedron: Asymmetry, 6(7), 1641-56; 1995

L3 ANSWER 45 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

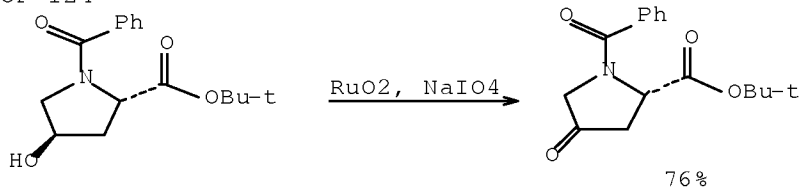
RX(29) OF 826



REF: PCT Int. Appl., 9523608, 08 Sep 1995
NOTE: mol. sieves used

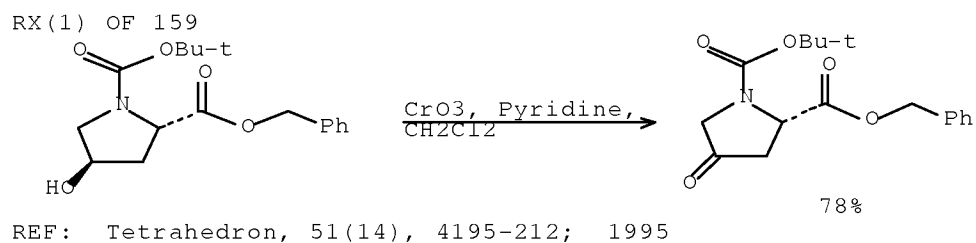
L3 ANSWER 46 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 124

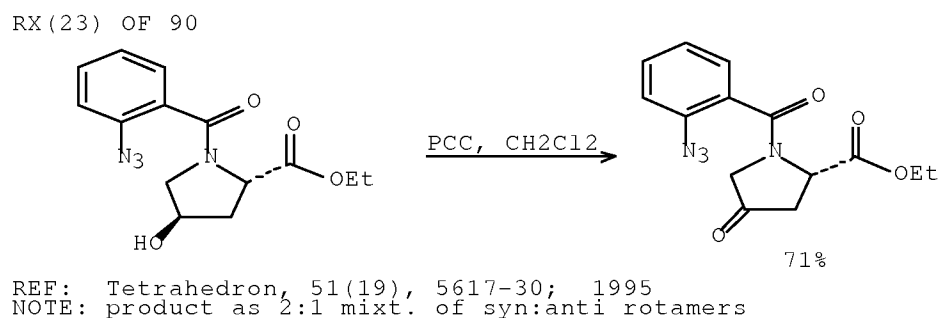


REF: Tetrahedron Letters, 36(27), 4869-72; 1995

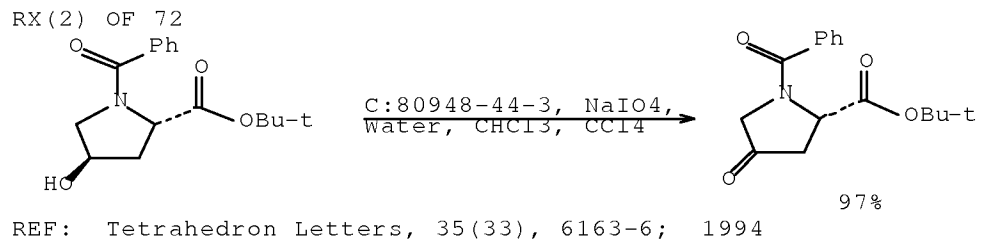
L3 ANSWER 47 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



L3 ANSWER 48 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

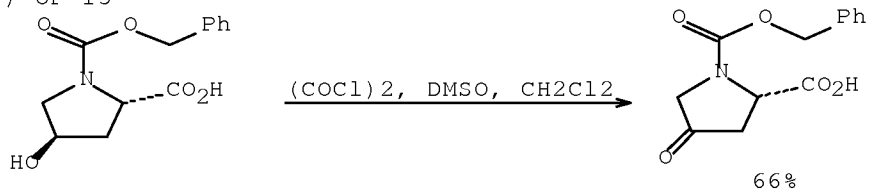


L3 ANSWER 49 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



L3 ANSWER 50 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

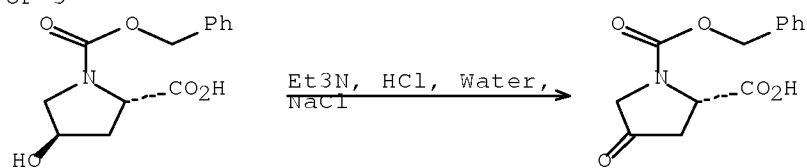
RX(1) OF 15



REF: Journal of Organic Chemistry, 57(19), 5264-8; 1992

L3 ANSWER 51 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

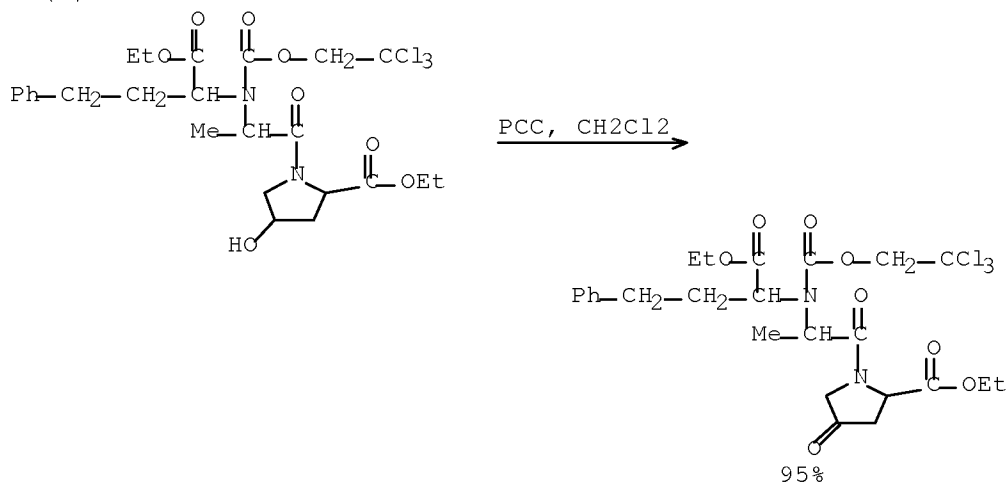
RX(1) OF 3



REF: Ger. (East), 283626, 17 Oct 1990

L3 ANSWER 52 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

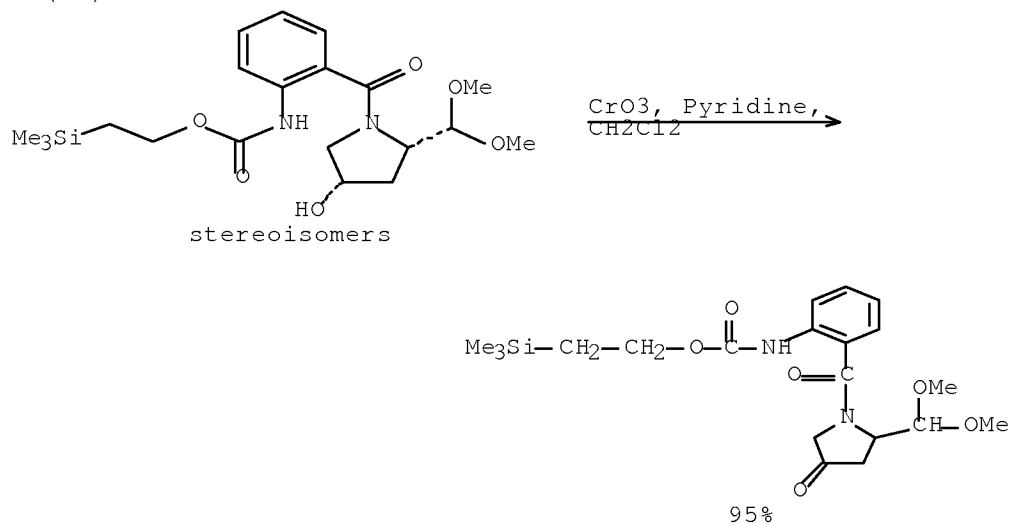
RX(2) OF 94



REF: Journal of Medicinal Chemistry, 33(6), 1606-15; 1990

L3 ANSWER 53 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

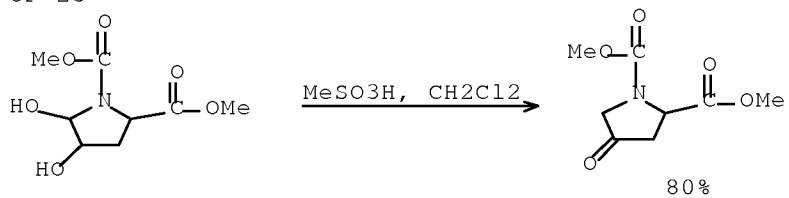
RX(29) OF 373



REF: Journal of Organic Chemistry, 54(24), 5746-58; 1989

L3 ANSWER 54 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

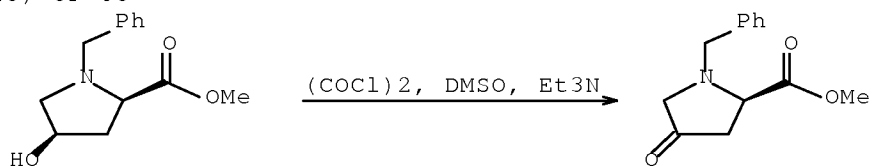
RX(11) OF 23



REF: Tetrahedron, 44(17), 5441-9; 1988

L3 ANSWER 55 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

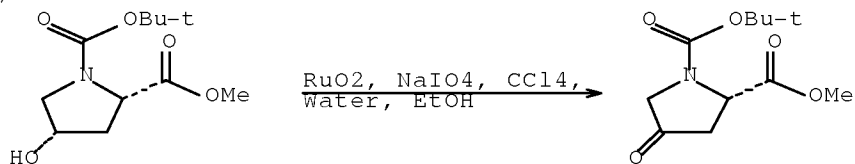
RX(13) OF 60



REF: Synthesis, (1), 40-4; 1988

L3 ANSWER 56 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

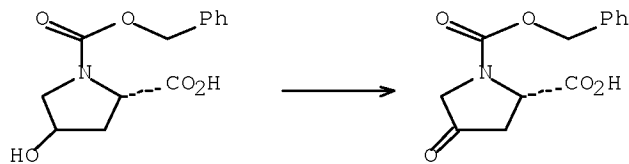
RX(1) OF 15



REF: Synthesis, (1), 81-2; 1986

L3 ANSWER 57 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

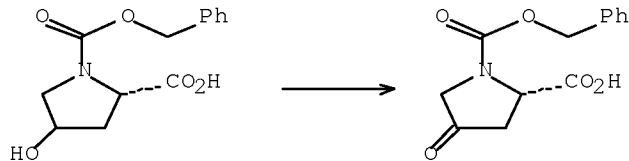
RX(2) OF 15



REF: U.S., 4311697, 19 Jan 1982

L3 ANSWER 58 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

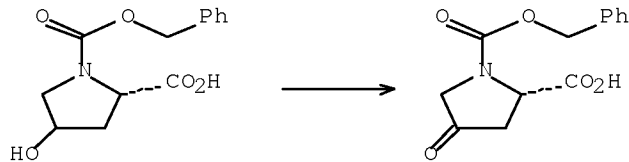
RX(1) OF 28



REF: U.S., 4296113, 20 Oct 1981

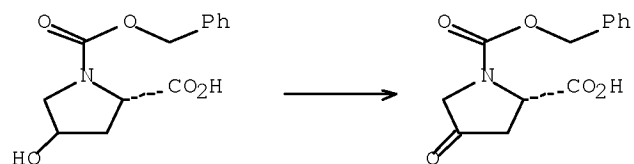
L3 ANSWER 59 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 10



REF: Ger. Offen., 3009684, 24 Sep 1981

RX(1) OF 9



REF: Belg., 882366, 22 Sep 1980

=> log hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.06

297.39

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 16:29:54 ON 14 APR 2008